Chloralose 15879-93-3 | DTXSID4020088

Model Performance						
	Model	Da	ata			

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 5.55e-01

Global applicability domain: Inside

Local applicability domain index: 4.73e-01

Confidence level: 5.62e-01

Nearest Neighbors from the Training Set

Image not found

Chloralose

Measured: 1.02 Predicted: 5.55e-01 Image not found

NSC226971

Measured: -0.630 Predicted: -0.623 Image not found

Isopropyl beta-D-1thiogalactopyranoside

Measured: -1.26 Predicted: -1.16